bio-protocol Preprint

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Molecular dynamics simulations

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An abbreviated version of this protocol was published in eLIFE in May 2020

Conformational distributions of isolated myosin motor domains encode their mechanochemical properties

DOI: 10.7554/eLife.55132

Detailed protocol

Thanks for your interest in our work! Apologies for the delayed response. We've been focused on COVID (both research and the personal implications) and are slowly catching up on other important tasks.

We've shared the starting structures for our simulations, the MSMs we constructed from the simulation data, and the code for performing PCA on the p-loops of these motors here:
https://osf.io/54g7p/

The rest of our analysis code, with examples, can be found here:
https://github.com/bowman-lab/enspara

How to cite:(Readers should cite both the Bio-protocol preprint and the original research article where this protocol was used)

1. Bowman, G. (2020). Molecular dynamics simulations. Bio-protocol Preprint. bio-protocol.org/prep443.
2. Porter, J. R., Meller, A., Zimmerman, M. I., Greenberg, M. J. and Bowman, G. R.(2020). Conformational distributions of isolated myosin motor domains encode their mechanochemical properties. eLIFE. DOI: 10.7554/eLife.55132